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CONDITIONS IN NUMERICAL SOLUTION
OF SYSTEMS OF NONLINEAR EQUATIONS
OF BOUNDARY-LAYER TYPE

by Philip R. Nachtsheim and Paul Swigert

Lewis Research Center

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SUMMARY

A method for the numerical solution of differential equations of the boundary-layer type is presented. The asymptotic boundary conditions are satisfied at the edge of the boundary layer by adjusting the initial conditions so that the mean square error between the computed variables and the asymptotic values is minimized. Convergence to a solution is rapid and appears to be insensitive to the initial guesses of the initial conditions. Use of a least-squares convergence criterion leads to the unique solution even in the case of retarded main stream flows. A description of the method is given, and two examples taken from boundary-layer theory are worked. For the Falkner-Skan differential equation, the relation between the wedge angle and the shear stress at the wall is obtained.

INTRODUCTION

The numerical integration of the ordinary differential equations of boundary-layer theory involves the satisfaction of asymptotic boundary conditions; that is, some boundary conditions are specified at the initial point or wall, and others are specified as limits that must be approached at large values of the independent variable corresponding to the edge of the boundary layer. In order to integrate the differential equations numerically from the wall to the edge of the boundary layer, it is necessary to specify as many additional conditions at the wall as there are conditions to be satisfied at the edge of the boundary layer. These additional initial conditions have to be varied in order to satisfy the conditions at the edge of the boundary layer. All methods that have been used to find the proper initial conditions rely on the fact that, for large values of the independent variable, the integrals of the differential equations depend on the initial conditions. One method that has been used to find the proper initial conditions, called the initial-value method (ref. 1), is that of obtaining integrals of the differential equations with guessed initial conditions; that is, an attempt is made to integrate the differential equations to

the edge of the boundary layer. If this can be accomplished, corrections are made for the initial guesses by the Newton-Raphson method, and the process is repeated until convergence is achieved.

In order to carry out this iteration, additional differential equations have to be integrated. The additional differential equations are obtained by differentiating the terms of the original differential equation with respect to the initial conditions. The integrals of these additional differential equations, henceforth referred to as perturbation equations, give the rate of change of the integrals of the original differential equation with respect to the initial conditions.

Another method that has been used, called quasilinearization (ref. 2), is similar in principle to the initial-value method, except that the original differential equations are linearized. The resulting linear differential equations for the current approximation are inhomogeneous, since they also contain the previous approximation as members.

The integrals of the perturbation equations of the initial-value method correspond to a complementary solution of the linear differential equations of the quasilinearization method. In application, the two methods are different in that, in the quasilinearization method, the complementary solutions are used to obtain solutions to the inhomogeneous linear differential equations, whereas in the initial-value method, the integrals of the perturbation equations are used to adjust the starting values at the initial point. A disadvantage associated with the quasilinearization method is that functions representing the previous approximation have to be stored in order to construct the current approximation. Furthermore, the solution of the inhomogeneous equation obtained by combining complementary solutions and a particular integral is usually not well determined except near the origin or initial point, as pointed out by Hartree (ref. 3). The solutions of the perturbation equations, however, can be used to determine the proper initial conditions closely. This is the procedure that is followed in the initial-value method.

Both methods have been used to obtain solutions of the boundary-layer equations. Neither of these methods, however, has solved the problem of when to stop the integration. Since one boundary condition is specified as a limit that must be approached at large values of the independent variable, the integration should be stopped at a value of the independent variable that is sufficiently large so that the various functions are approaching their asymptotic values. This value of the independent variable could properly be called the edge of the boundary layer. In the various methods used to solve this problem, this value of the independent variable must be guessed beforehand. If the guessed value is too small, the integrals of the differential equation may not be able to satisfy the imposed conditions; or, there may be more than one value of an initial condition that leads to integrals of the differential equations that satisfy the imposed boundary conditions.

If the guessed value is too large, it is possible that the integrals of the equations

will diverge, or that convergence to a solution is extremely slow.

Another problem that sometimes besets the numerical integration of the boundary-layer equations is the apparent insensitivity of the integrals of the boundary-layer equations to the initial conditions. This difficulty appears in the integration of the Falkner-Skan differential equation (ref. 4). All the integrals of the Falkner-Skan equation for the case of nonretarded flows in the main stream tend to diverge except the ones with the proper initial conditions; however, for the case of retarded flows, a solution with any value of the initial condition near the correct one will eventually meet the proper boundary condition at infinity. The unique solution was found by Hartree (ref. 4) for retarded flows by imposing the additional condition that the desired solution is the one that approaches the boundary condition most rapidly from below. However, this behavior of the solutions can only be learned from several trial runs.

In an effort to adapt the initial-value method to the solution of differential equations with asymptotic boundary conditions, a method was developed to eliminate the problem of when to stop the integration. This method of solution is capable of satisfying the boundary conditions at the edge of the boundary layer correctly; that is, the boundary values are approached asymptotically. This is accomplished by choosing the additional initial conditions so that the mean square error between the computed variables and the asymptotic values is minimized. A method of solution is proposed that is based on a least-squares convergence criterion in which the edge of the boundary layer is approached in steps. The convergence rate to a solution is rapid, and convergence appears to be insensitive to the initial guesses of the initial conditions. Use of a least-squares convergence criterion leads to the unique solution even in the case of retarded main stream flows. A description of the method is given, and two examples taken from boundary-layer theory are worked. By using this method of solution it is feasible to obtain directly, for those differential equations which contain a parameter, the relation between the properties of the solutions and the values of the parameter. For the Falkner-Skan differential equation, the relation between the wedge angle and the shear stress at the wall is obtained.

DESCRIPTION OF METHOD

A description of the method can best be given by referring to a definite example of a boundary-value problem with an asymptotic boundary condition. In Falkner and Skan's treatment of the laminar boundary layer of an incompressible fluid, the following equation arises (see ref. 4):

$$f''' = -ff'' + \beta(f'^2 - 1) \quad (1)$$

with the boundary conditions

$$\eta = 0: f = f' = 0$$

$$\eta \rightarrow \infty: f' \rightarrow 1$$

(Symbols are defined in appendix A.) Primes denote differentiation with respect to η , a measure of the distance from the wall. The dependent variable f is related to the usual stream function. The potential flow is given by a power law. The flow velocity outside the boundary layer in the main stream is proportional to the distance along the wall raised to the power $\beta/(2 - \beta)$. For retarded main stream flow $\beta < 0$, and for non-retarded flow $\beta \geq 0$.

In practice, the asymptotic boundary condition is replaced by the condition that $f' = 1$ to a sufficient degree of accuracy at $\eta = \eta_{\text{edge}}$, where η_{edge} is the value of the independent variable at the edge of the boundary layer. The boundary-value problem is equivalent to the problem of finding a value of $f''(0)$ for which the boundary condition at the edge of the boundary layer is satisfied; that is, it is desired to find a solution of the nonlinear equation

$$f'_{\text{edge}}[f''(0)] = 1$$

where $f'_{\text{edge}} \equiv f'(\eta_{\text{edge}})$. The function $f'_{\text{edge}}[f''(0)]$ in this problem is not, in general, explicit; it will be expressed as a function of $f''(0)$ through an integration of equation (1). With the notation $x \equiv f''(0)$, observe that a small change Δx in x changes f' by the amount

$$\frac{\partial f'}{\partial x} \Delta x$$

so that the necessary correction to a first approximation comes from the solution of the linear equation

$$1 = f' + \frac{\partial f'}{\partial x} \Delta x$$

at $\eta = \eta_{\text{edge}}$.

The solution of the equation for Δx can be performed provided that the partial derivative of f' with respect to x can be evaluated at η_{edge} . The partial derivative can be evaluated by forming the perturbation equation for the function f' . This equation

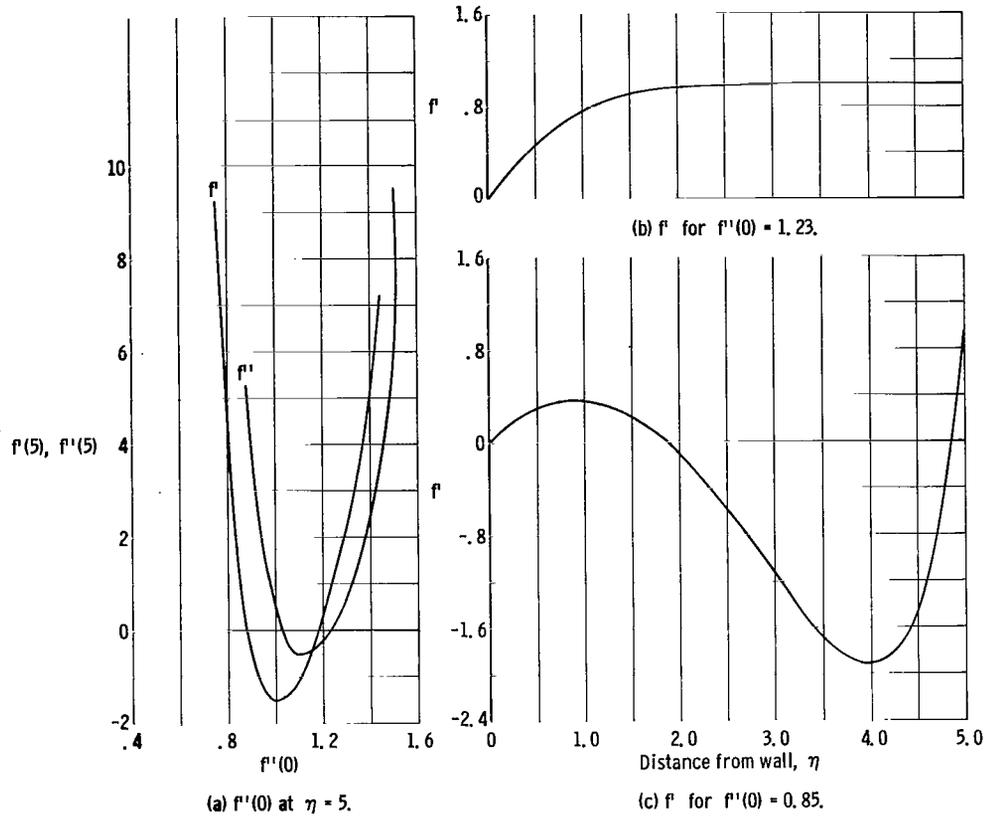


Figure 1. - Variation of f' and f'' . Falkner-Skan parameter, L .

is obtained by differentiating the terms in equation (1) appropriately. With the notation

$$f_x = \frac{\partial f}{\partial x}, \quad f'_x = \frac{\partial f'}{\partial x}, \quad \dots$$

the following perturbation equation is obtained:

$$f'''_x = -(ff''_x + f''f'_x) + 2\beta f'_x f'_x \quad (2)$$

with the initial conditions

$$\eta = 0: \quad f_x = f'_x = 0, \quad f''_x = 1$$

Given an initial estimate of $x = f''(0)$, subsequent values of x can be computed by integrating equations (1) and (2) and applying the Newton-Raphson method to obtain corrections.

The problem of where to stop the integration remains; that is, η_{edge} is unknown. Figure 1(a) illustrates the difficulties that arise when the boundary condition $f' = 1$ is

applied at a finite value of η . The data for figure 1(a) were obtained by integrating equation (1) for specified values of $f''(0)$ with $\beta = 1$. The integration was stopped at $\eta = 5$. Tentative values of η_{edge} will hereinafter be referred to as η_{stop} . It should be noted that the problem is not that η_{edge} is unknown, but an appropriate η_{stop} must be determined in some fashion for use in the as yet unconverged iterations.

Figure 1(a) shows f' and f'' as a function of $x = f''(0)$ at $\eta_{\text{stop}} = 5$. It can be seen that there are two values of x that satisfy the condition $f' = 1$ when η_{stop} is taken to be 5, namely, approximately $x = 0.85$ and $x = 1.23$. Figures 1(b) and (c) show the two solutions corresponding to the two values of x . It can be concluded from this illustration that the satisfaction of the single boundary condition $f' = 1$ at $\eta_{\text{stop}} = 5$ does not lead to a unique solution. The proper value of x can be determined by observing where $f'' = 0$. From figure 1(a) it can be seen that the correct value of x is approximately 1.23. Satisfaction of both boundary conditions $f' = 1$ and $f'' = 0$ at $\eta_{\text{stop}} = 5$ ensures the satisfaction of the original boundary condition of f' , namely, that f' approaches unity asymptotically as η approaches infinity. Hence, in order to satisfy the asymptotic condition at a finite value of η , the conditions $f' = 1$ and $f'' = 0$ should both be imposed (examination of the differential equation, (eq. (1)), will reveal that all higher derivatives will be zero also); that is, Δx should be chosen so that both equations

$$1 = f' + f'_x \Delta x \quad (3)$$

and

$$0 = f'' + f''_x \Delta x \quad (4)$$

are satisfied at $\eta = \eta_{\text{stop}}$. This is, in general, impossible since there are two conditions and only one adjustable parameter Δx . However, a satisfactory solution that is consistent with the idea that the boundary condition cannot be satisfied exactly at a finite value of η is to seek the least-squares solution of equations (3) and (4) (ref. 5). Hence consider the discrepancies δ_1 and δ_2 , where

$$\delta_1 = f'_x \Delta x + f' - 1$$

$$\delta_2 = f''_x \Delta x + f''$$

and attempt to find a value for Δx that will make the sum $\delta_1^2 + \delta_2^2$ as small as possible. To minimize the sum, it is necessary to equate its first derivative with respect to Δx to zero. This calculation yields a value of Δx corresponding to the minimum of the sum $\delta_1^2 + \delta_2^2$, that is,

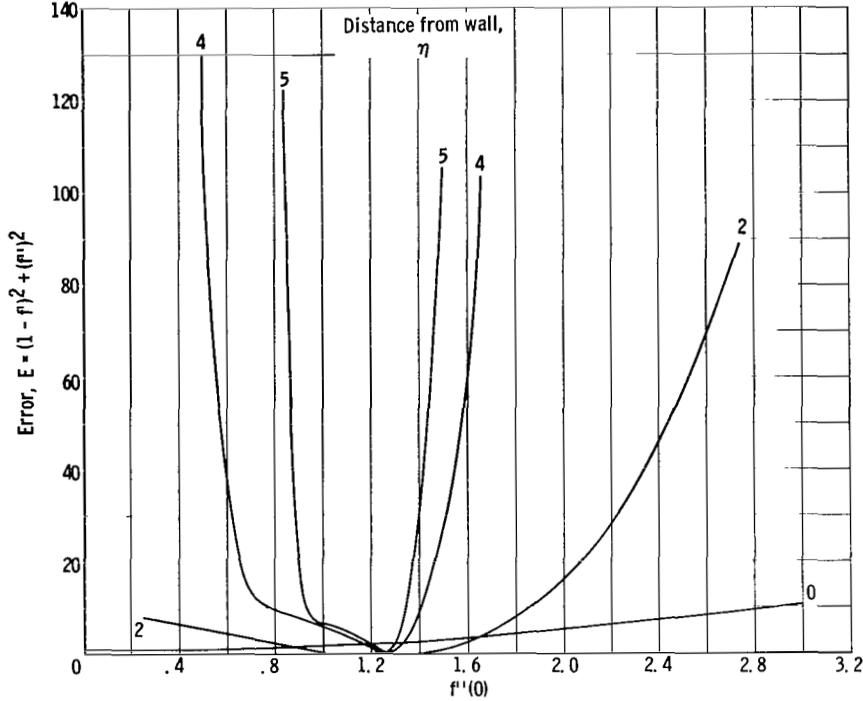


Figure 2. - Error as function of $f''(0)$ for different values of η_{stop} . Falkner-Skan parameter, 1.

$$\Delta x = \frac{f'_x(1 - f') - f''_x f''}{f'_x{}^2 + f''_x{}^2} \quad (5)$$

Along with the discrepancies δ_1 and δ_2 consider the sum of the squares of the deviations of the computed quantities from their asymptotic values

$$E = (1 - f')^2 + f''^2 \quad (6)$$

Henceforth, E shall be referred to as the error. The magnitude of E evaluated at η_{stop} gives an indication of how unsatisfactory the asymptotic boundary conditions are. The value of x that gives $\Delta x = 0$ corresponds to the minimum with respect to x of E , as can be seen from equation (5). In figure 2, the quantity E is shown plotted as a function of x for various values of η_{stop} . The data for figure 2 were also obtained from the integrations that were used to prepare figure 1. It can be seen that the least-squares solution gives a unique solution for x . It is this property, that the minimum of E with respect to x , E_{min} , corresponds to no change in the required initial conditions, that permits the asymptotic boundary condition to be approximately satisfied at a finite value of the independent variable.

For this example, the Falkner-Skan solution with $\beta = 1$, it appears that the quantity

E has a definite minimum at each value of η , even at $\eta = 0$, as seen from figure 2. The edge of the boundary layer could be defined as that value of η for which the value of E_{\min} is less than some preassigned small value as the range of integration is increased. This gives a value of η_{edge} .

The concept of convergence in the least-squares sense allows the initial-value method to be modified in order to solve a wide class of boundary-layer problems. To understand why the initial-value method requires modification, consider how the method can fail when it is applied to boundary-layer-type problems.

Recall that in the initial-value method corrections are obtained to the guessed initial conditions after integrating the differential equations to the edge of the boundary layer. This method can fail if the initial guess is so poor that the integration "blows up" (i. e., diverges beyond a prescribed limit) before reaching the edge of the boundary layer.

This problem can be avoided and corrections to the initial conditions can be obtained by attempting to minimize the mean square error between the computed solution and the asymptotic values before reaching the edge of the boundary layer. The modification of the initial-value method consists then of finding E_{\min} at any arbitrary value of η_{stop} . By this modified procedure, the choice of η_{stop} , where the minimizing process is first carried out, may be dictated by other considerations than where the edge of the boundary layer is, such as keeping the variables within prescribed limits so that the solution does not diverge. After E_{\min} has been found, no further corrections to the initial conditions need to be made at the chosen value of η_{stop} , and the range of integration can be increased if necessary.

If the value of E_{\min} found is not small enough, it will be necessary to increase the range of integration. In this way, the edge of the boundary layer is approached in steps by successively increasing the range of integration until the correct initial conditions and the value of η_{edge} are found. In other words, as η_{stop} is increased, E_{\min} tends to zero, and the required initial condition $x = f''(0)$ also tends to a definite value. This gives the solution of the boundary-value problem.

NUMERICAL SOLUTION

The method described in the previous section was programed in FORTRAN IV, double precision on the IBM 7094II-7040 direct-couple system. The boundary-layer and perturbation differential equations were rewritten as systems of first-order differential equations and integrated with a predictor-corrector (Adams-Moulton) subroutine using one correction per step and a fixed increment.

The boundary-layer equations along with the perturbation equations were integrated

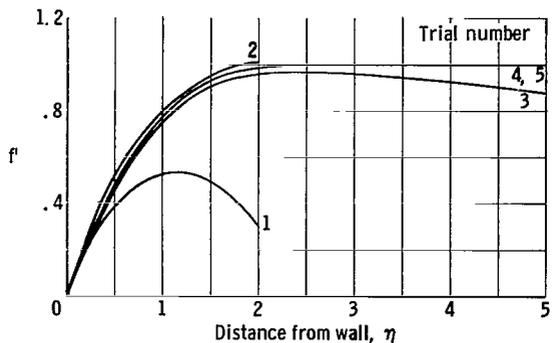


Figure 3. - Convergence history of solution of equation (1) Falkner-Skan parameter, 1.

to the specified value of the independent variable. The corrections were then determined, and the process was repeated until the relative change in the correction term, equation (5), was less than a small preassigned value.

Extreme accuracy was not required at the smaller values of η_{stop} since the boundary conditions cannot be well satisfied there. A value of 1×10^{-8} was used at the larger values of η_{stop} to check the relative change in the correction term. This small value seemed reasonable since convergence is so rapid.

RESULTS OF NUMERICAL SOLUTION FOR EXAMPLE 1

Figure 3 shows the solution f' of equation (1) with $\beta = 1$ as a function of the independent variable η , for the five trials needed for convergence. With an initial guess of 1.0 for $f''(0)$, the equations were integrated to a value of $\eta_{stop} = 2$ twice and to a value of $\eta_{stop} = 5$ three times. Observe that, for the first integration, the values of f' tend to deviate radically from the correct solution at a relatively small value of η . If these calculations had been carried out to a larger value of η , the values of f' would have attained a magnitude so large that any use of these large numbers in a Newton-Raphson scheme would be meaningless.

TABLE I. - EFFECT OF η_{stop} ON CONVERGENCE RATE

$f''(0)$ (initial guess)	$\eta_{stop} = 2$		$\eta_{stop} = 5$	
	$f''(0)$ (after two trials)	Percent difference	$f''(0)$ (after two trials)	Percent difference
0.25	1.2799034	3.83	0.26706180	-78.33
.50	1.2449846	1.00	.69205364	-43.85
.75	1.2292604	-.26	.88486032	-28.21
1.00	1.2266764	-.47	1.0413712	-15.51
1.25	1.2266282	-.48	1.2325888	.00
1.50	1.2266765	-.47	1.2444813	.96
1.75	1.2277231	-.39	1.2890732	4.58
2.00	1.2312423	-.10	1.3564389	10.04
2.25	1.2383960	.47	1.8834930	52.80
2.50	1.2498889	1.40	2.4946776	102.39
2.75	1.2660459	2.71	-----	-----
3.00	1.2869264	4.40	-----	-----

TABLE II. - CONVERGENCE HISTORY OF INITIAL VALUES

(a) Example 1

Trial	Correction	η_{stop}	$f''(0)$
1		2.0	1.0
2	1	2.0	1.2463981
3	2	5.0	1.2266764
4	3	5.0	1.2326729
5	4	5.0	1.2325878
	5		1.2325878
Literature values			
Source	η_{stop}	$f''(0)$	
Ref. 2	5.0	1.2397	
Ref. 6	4.0	1.2325876	

(b) Example 2

Trial	Correction	η_{stop}	$f''(0)$	$h'(0)$
1		2.0	1.0	-1.0
2	1	2.0	.61735605	-.59008297
3	2	8.0	.63211384	-.57655550
4	3	8.0	.66795925	-.52593128
5	4	8.0	.67387305	-.50916398
6	5	8.0	.67412049	-.50790411
7	6	8.0	.67412438	-.50789273
	7		.67412438	-.50789273
Literature values				
Source	η_{stop}	$f''(0)$	$h'(0)$	
Ref. 8	8.0	0.6741	-0.5080	

The effect of η_{stop} on the convergence process is illustrated in figure 2 and table I. Figure 2 shows the error, equation (6), as a function of $f''(0)$ for different values of η_{stop} . Observe that by initially using a small value for η_{stop} ($\eta_{stop} = 2$ in fig. 2) the range of meaningful initial guesses is increased, that is, initial guesses that yield a relatively small error. For extremely large values of η_{stop} the parabola-like curves in figure 2 degenerate to a vertical line, and the initial guess is limited to the correct answer.

Table I shows the effect of η_{stop} on the convergence rate. Also, the values of $f''(0)$ after two trials and the percentage difference from the correct value of $f''(0)$ for a wide range of initial guesses and two values of η_{stop} are given. The convergence to the correct answer is always faster for the smaller η_{stop} except when the initial guess is close to the correct answer. In fact, the two largest initial guesses "overflowed" the computer before the larger η_{stop} was reached. This indicates that a very crude initial guess may be used if the integration is carried out to a small η_{stop} .

To give an idea of the rate of convergence to a solution for this example using an initial guess of $f''(0) = 1$, table II(a) is presented. Using quasilinearization and five corrections, Radbill (ref. 2) obtained a value of $f''(0)$ that agrees with that of Yohner and Hansen (ref. 6) to within seven units in the third decimal place. The method developed herein reached an answer after two corrections that agrees with that of Yohner and Hansen to within six units in the third decimal place. After two more corrections the answer agreed to within two units in the seventh decimal place (see table II(a)). The last integration was performed as a stopping criterion for the computer. Computer time for the complete solution, using a step size of 2^{-4} was approximately 0.03 minute.

This example was also programmed by single precision with good results. The

difficulty in using single precision presented itself in the form of reducing the range of initial guesses that yielded a relatively small error. Evidently, this was caused by the increased round-off error associated with the use of single precision.

Equation (1) was also integrated for the case of a retarded main stream flow with $\beta = -0.1$. However, no additional conditions such as those used by Hartree (ref. 4) had to be imposed in order to obtain the unique solution. The value of $f''(0)$, which was obtained by minimizing the mean square error, agreed with the value obtained by Smith (ref. 7) for this case to six decimal places. A description of the flow chart and the FORTRAN listing for this program are presented in appendix B.

EXTENSION TO SYSTEMS OF EQUATIONS

The least-squares modification of the initial-value method described in the preceding section for a differential equation with a single dependent variable can easily be generalized to systems of equations. As an example of a problem with two dependent variables, consider the boundary-value problem for the free-convection flow about a vertical plate. This example is taken from reference 8. It consists of solving the differential equations

$$f''' = -3ff'' + 2f'^2 - h \quad (7)$$

$$h'' = -3Prfh' \quad (8)$$

with the boundary conditions

$$\eta = 0: f = f' = 0, h = 1$$

$$\eta \rightarrow \infty: f' \rightarrow 0, h \rightarrow 0$$

Again the primes denote differentiation with respect to η (a measure of the distance from the wall), and the dependent variable f is a dimensionless form of the usual stream function. The dependent variable h is proportional to the temperature excess of the fluid over the ambient temperature, and Pr denotes the Prandtl number.

Since there are two asymptotic boundary conditions to satisfy, two additional initial conditions at the wall will have to be adjusted; that is, values of $x \equiv f''(0)$ and $y \equiv h'(0)$ are sought that will satisfy simultaneously the nonlinear equations.

$$h_{\text{edge}}[f''(0), h'(0)] = 0$$

and

$$f'_{\text{edge}}[f''(0), h'(0)] = 0$$

where $f'_{\text{edge}} \equiv f'(\eta_{\text{edge}})$ and $h_{\text{edge}} \equiv h(\eta_{\text{edge}})$. The necessary first corrections to a first approximation x and y come from a solution of the linear equations

$$0 = f' + f'_x \Delta x + f'_y \Delta y$$

and

$$0 = h + h_x \Delta x + h_y \Delta y$$

at $\eta = \eta_{\text{edge}}$, where $f'_x = \partial f' / \partial x$, $f'_y = \partial f' / \partial y$, etc. However, in order to satisfy the asymptotic boundary conditions, the preceding equations must be supplemented by

$$0 = f'' + f''_x \Delta x + f''_y \Delta y$$

and

$$0 = h' + h'_x \Delta x + h'_y \Delta y$$

and Δx and Δy must be found such that the sum of squares of the errors in the preceding four equations be a minimum. The least-squares solution for those quantities is given by the solution of the following matrix equation:

$$\begin{bmatrix} f_x'^2 + h_x^2 + f_x''^2 + h_x'^2, & f'_x f'_y + h_x h_y + f_x'' f_y'' + h_x' h_y' \\ f'_x f'_y + h_x h_y + f_x'' f_y'' + h_x' h_y', & f_y'^2 + h_y^2 + f_y''^2 + h_y'^2 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = - \begin{bmatrix} f'_x f'_x + h h_x + f'' f_x'' + h' h_x' \\ f'_y f'_y + h h_y + f'' f_y'' + h' h_y' \end{bmatrix} \quad (9)$$

The values of x and y that give $\Delta x = \Delta y = 0$ correspond to the minimum with respect to x and y of the quantity

$$E = f'^2 + h^2 + f''^2 + h'^2 \quad (10)$$

The partial derivatives with respect to x and y that appear in equation (9) are obtained by integrating the appropriate perturbation differential equations. The perturbation differential equations for the x derivatives are

$$f_x''' = -3(f_x f_x'' + f f_x'') + 4f'_x f'_x - h_x \quad (11)$$

and

$$h_x'' = -3Pr(f_x h' + f h_x') \quad (12)$$

with the initial conditions

$$\eta = 0: f_x = f'_x = h_x = h'_x = 0; f_x'' = 1$$

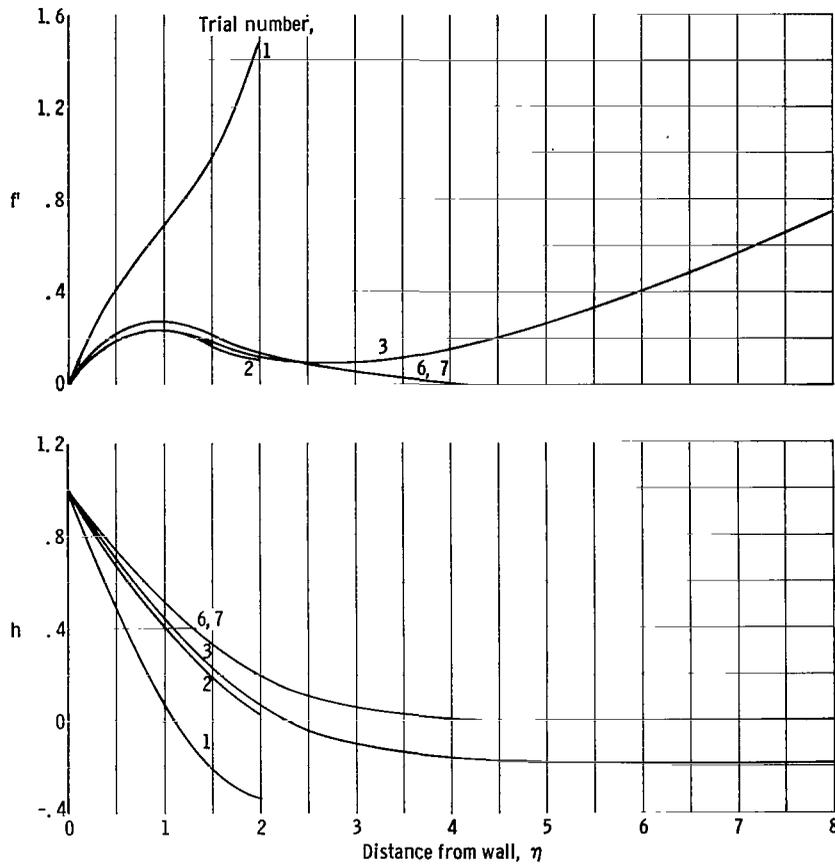


Figure 4. - Convergence history of solutions of equations (7) and (8). Prandtl number, 0.733.

The perturbation differential equations for the y derivatives are

$$f_y''' = -3(f_y f'' + f f_y'') + 4f' f_y' - h_y \quad (13)$$

and

$$h_y'' = -3Pr(f_y h' + f h_y') \quad (14)$$

with the initial conditions

$$\eta = 0: f_y = f_y' = f_y'' = h_y = 0; h_y' = 1$$

Note that the equations for the y derivatives are the same as the equations for the x derivatives. The integrals of these equations will differ since the initial conditions are different.

Note also that there are as many additional systems of perturbation equations to

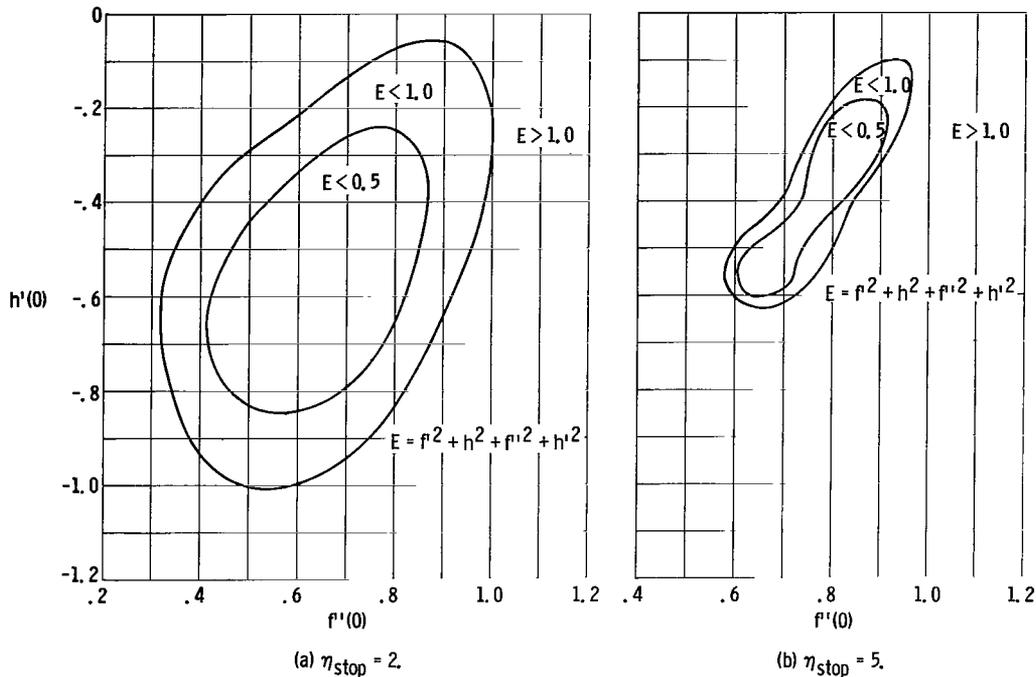


Figure 5. - Level curves of error against $f'(0)$ and $h'(0)$.

integrate as there are asymptotic boundary conditions to meet.

NUMERICAL SOLUTION OF CONVECTIVE FLOW PROBLEM FOR EXAMPLE 2

The same general procedure used in the previous example was employed to solve this example. One notable difference is that five trials were needed at the larger value of η_{stop} , rather than the three trials of the first example. This is probably because of the need of adjusting two initial conditions rather than one and because an error in one initial condition leads to an error in computing the correction term of the other.

The solutions of equations (7) and (8) are shown in figure 4 for $Pr = 0.733$. Note (as in the previous example) that the functions f' and h of figure 4 diverge radically from the true solutions, for the initial guesses of trial 1.

Table II(b) (p. 10) shows the rapid rate of convergence for this more difficult example. With initial guesses of 1.0 and -1.0 for $f'(0)$ and $h'(0)$, respectively, convergence is realized after two trials with $\eta_{\text{stop}} = 2$ and five trials with $\eta_{\text{stop}} = 8$. The results are in close agreement with the published values of Ostrach (ref. 8).

The effect of η_{stop} on the convergence process for this example is illustrated in figures 5(a) and (b). Level curves for the error, equation (10), are plotted in the $f'(0), h'(0)$ plane for $\eta_{\text{stop}} = 2$ in figure 5(a), and for $\eta_{\text{stop}} = 5$ in figure 5(b). As in the previous example, by using a small value for η_{stop} , the range of initial guesses

that yields a relatively small error is again increased; that is, the area where E is less than 1 is much greater in figure 5(a) than in figure 5(b). For extremely large values of η_{stop} , that is, η_{stop} greater than 8, the area enclosed by the level curve where E is less than 1 shrinks to a point, and the initial guess is limited to the correct answer.

Computer time for the second example was about 0.10 minute with a step size of 2^{-4} . In both examples, the convergence was made insensitive to the initial guesses by choosing a small value of η_{stop} for the first two trials. The answer thus obtained for the initial conditions was good enough so that η_{stop} could be increased considerably. The error term may be made as small as desirable by continuous extension of the range of integration. This error term may also be used as a stopping criterion for computer calculations and finding η_{edge} automatically. A discussion of the flow chart and the FORTRAN listing for this program are given in appendix B.

SOLUTIONS OF AN EQUATION CONTAINING A PARAMETER

Very often it is desired to examine the general properties of the solutions of a differential equation containing a parameter when the parameter is varied. For example, in the case of the Falkner and Skan differential equation (eq. (1)), which contains the parameter β , it is desirable to know the variation of $f''(0)$ with β . The physical significance of $f''(0)$ is that it is proportional to the shear stress at the wall.

If $\beta > 0$, the flow may be regarded as that near a wedge, and the included angle of the wedge is $\beta\pi$. But if $\beta < 0$, it can only be said that it corresponds to a flow in an adverse pressure gradient (retarded main stream flow). It is desired to know the behavior of the shear stress as β is varied. It is especially important to know what value of β gives $f''(0) = 0$, that is, the laminar separation profile. This behavior of the solutions can be learned by solving equation (1) for a preassigned set of values of β and determining a set of values of $f''(0)$.

Since the modification of the initial-value method described previously allows accurate solutions of equation (1) to be obtained quickly and easily, it is feasible to obtain the variation of $f''(0)$ with β by using a more economical procedure than by obtaining solutions for a preassigned set of values of β . This procedure is essentially the method of steepest descent, as explained in reference 9. It consists of finding the curve of solutions $f''(0)$ against β in the $\beta, f''(0)$ plane and following it. The points that lie on the curve of solutions are the values that allow equation (1) to satisfy the imposed boundary conditions.

The curve of solutions of equation (1) in the $\beta, f''(0)$ plane can be considered to be given implicitly by the equation

$$f'_{\text{edge}}[\beta, f''(0)] = 1 \quad (15)$$

where $f'_{\text{edge}} \equiv f'(\eta_{\text{edge}})$. Any point $\beta, f''(0)$ in the plane may be regarded as lying on a curve $f'_{\text{edge}} = \text{constant}$. If $\beta, f''(0)$ is an approximate solution of equation (15), the curve $f'_{\text{edge}} = \text{constant}$ will be nearly parallel to the curve of solutions $f'_{\text{edge}} = 1$, and the necessary corrections to a first approximation can be found by solving the equation

$$1 = f' + f'_{\beta} \Delta\beta + f'_{\text{x}} \Delta x \quad (16)$$

together with the equation

$$0 = -f'_{\text{x}} \Delta\beta + f'_{\beta} \Delta x \quad (17)$$

at $\eta = \eta_{\text{edge}}$, where $f'_{\beta} = \partial f' / \partial \beta$ and $f'_{\text{x}} = \partial f' / \partial x$, $x \equiv f''(0)$. Equation (17) guarantees that the increment $(\Delta\beta, \Delta x)$ will be perpendicular to the curves $f'_{\text{edge}} = \text{constant}$. Successive iterations lead to a point on the curve $f'_{\text{edge}} = 1$. The direction of the tangent can be obtained by solving

$$0 = f'_{\beta} + f'_{\text{x}} \frac{dx}{d\beta} \quad (18)$$

for $dx/d\beta$ and may then be used to predict further points close to the curve.

The solution of the equations for $(\Delta\beta, \Delta x)$ (eqs. (16) and (17)) can be performed provided that the partial derivatives of f' with respect to x and β can be evaluated at η_{edge} . The partial derivatives with respect to x can be obtained from the solution of equation (2), as explained previously. The partial derivatives for the β variation can be evaluated by forming the perturbation equation for the function f' . This equation is obtained by differentiating the terms in equation (1) appropriately with respect to β . The following perturbation equation for the β variation is obtained

$$f'_{\beta}{}'' = -(ff'_{\beta}{}'' + f''f_{\beta}) + 2\beta f'f'_{\beta} + (f'^2 - 1) \quad (19)$$

with the initial conditions

$$\eta = 0: f_{\beta} = f'_{\beta} = f'_{\beta}{}'' = 0$$

Note that equation (19) is an inhomogeneous differential equation so that the homogeneous initial conditions do not necessarily yield a trivial solution.

Furthermore, note that, if the requirement of steepest descent is dropped, for

example, that is, the curve of solutions is approached on a line parallel to the β -axis, equation (19) alone could be used in conjunction with equation (1) without the use of equation (2) to obtain the curve of solutions for preassigned values of $x = f''(0)$. In this way, the value of β that gives the separation profile $f''(0) = 0$ can be found.

The requirement of the asymptotic approach of the solutions to the proper values is incorporated by recognizing that the curve of solutions of equation (1) can also be considered to lie on the curve given implicitly by the equation

$$f''_{\text{edge}}[\beta, f''(0)] = 0 \quad (20)$$

and requiring that this equation, where $f''_{\text{edge}} = f''(\eta_{\text{edge}})$, be satisfied as well as equation (15) at $\eta = \eta_{\text{edge}}$. In this case, if $\beta, f''(0)$ is an approximate solution of equation (20), the necessary corrections to a first approximation can be found by solving the equation

$$0 = f'' + f''_{\beta} \Delta\beta + f''_{\text{x}} \Delta x \quad (21)$$

together with the equation

$$0 = -f''_{\text{x}} \Delta\beta + f''_{\beta} \Delta x \quad (22)$$

at $\eta = \eta_{\text{edge}}$. The direction of the tangent can be obtained by solving

$$0 = f''_{\beta} + f''_{\text{x}} \frac{dx}{d\beta} \quad (23)$$

for $dx/d\beta$. The required values of $\Delta\beta, \Delta x$ for the asymptotic approach are obtained from the least-squares solution of equations (16), (17), (21), and (22). The least-squares solution for these quantities is given by

$$\Delta\beta = - \frac{f'_{\beta}(f' - 1) + f'_{\beta}f''}{f'_{\beta}{}^2 + f'_{\text{x}}{}^2 + f'_{\beta}{}^2 + f'_{\text{x}}{}^2} \quad (24)$$

and

$$\Delta x = - \frac{f'_{\text{x}}(f' - 1) + f'_{\text{x}}f''}{f'_{\beta}{}^2 + f'_{\text{x}}{}^2 + f'_{\beta}{}^2 + f'_{\text{x}}{}^2} \quad (25)$$

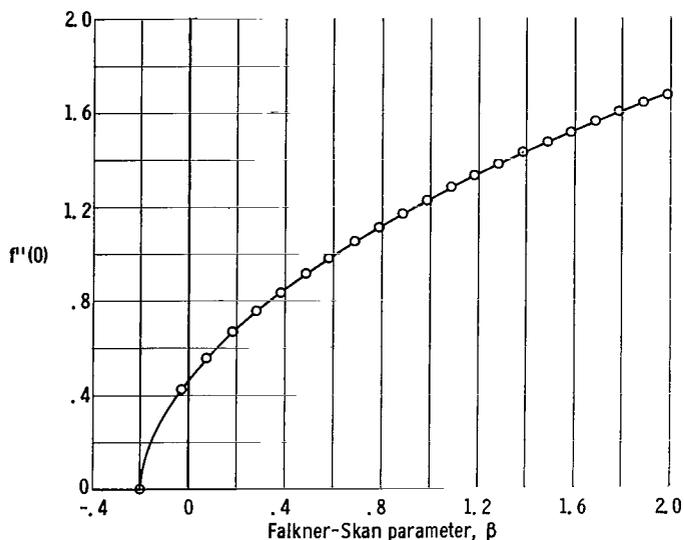


Figure 6. - Curve of solutions.

and the least-squares solution of equations (18) and (23) gives the direction of the tangent

$$\frac{dx}{d\beta} = - \frac{f'_x f'_\beta + f''_x f''_\beta}{f'^2_x + f''^2_x} \quad (26)$$

The process just described was programed for solution on the computer. Very few changes were needed in the program used in example 1. Appendix B gives a discussion and the FORTRAN listing of this program.

The entire curve of solutions (fig. 6), defined by 23 points over the range $\beta = -0.1$ to 2.1, was obtained in approximately 0.8 minute of computer time. Two values of η_{stop} were used for this solution; they are 4.0 and 8.0. The smaller η_{stop} was used only twice to start the solution since the predicted points on the curve of solutions, obtained from equation (26), were accurate enough to integrate directly to the larger η_{stop} . A solution was obtained in about four iterations, for each point, in this manner.

Equations (2) and (19) were integrated along with equation (1) to give the necessary terms for the corrections obtained from equations (24) and (25). When convergence was realized, equation (26) was applied to predict a new solution.

The value of β where $f''(0) = 0$ was obtained by the method of example 1 by treating β as the dependent variable; that is, $f''(0)$ was held constant, while β was allowed to vary. This is accomplished by integrating equation (19) along with equation (1) and applying the correction factor given by

$$\Delta\beta = \frac{f'_\beta(1 - f') - f''_\beta f''}{f'^2_\beta + f''^2_\beta}$$

Note the similarity to equation (5).

This method with $\eta_{\text{stop}} = 16$ yielded an error term (eq. (6)) of less than 1×10^{-28} . The numerical value of β when $f''(0) = 0$ is -0.198837682 and agrees with that of reference 7 to six decimal places. When the value of β presented in reference 7 was used in the program of example 1, the solution oscillated, and convergence could not be achieved. When the value presented herein was used, no such oscillation was experienced.

CONCLUSIONS

The two main problems of integrating the boundary-layer equations, namely, approximating the missing initial conditions and determining when to stop the integration in the as yet unconverged iterations, have been reduced to an automatic initial-value technique that is easily programed on high-speed computers. The technique was successfully applied to two problems taken from boundary-layer theory and offers promise of producing equivalent results when applied to other boundary-layer problems. The method appears to be insensitive to initial guesses and converges quickly to the solution. By this method the implicit study of differential equations containing a parameter has also been reduced to an automatic technique.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, June 11, 1965.

APPENDIX A

SYMBOLS

E	sum of squares of errors in boundary conditions	Subscripts:	
f	related to stream function	edge	edge of boundary layer
h	related to temperature excess of fluid over ambient temperature	stop	tentative values of edge of boundary layer
Pr	Prandtl number	x	denotes partial differentiation with respect to x
x	$x \equiv f'(0)$	y	denotes partial differentiation with respect to y
Δx	increment in x	β	denotes partial differentiation with respect to β
y	$y \equiv h'(0)$	Superscript:	
Δy	increment in y	'	denotes differentiation with respect to η
β	Falkner-Skan parameter		
$\Delta\beta$	increment in β		
η	measure of distance from wall		

APPENDIX B

DESCRIPTION OF FLOW CHART OF MAIN PROGRAM

A general flow chart (fig. 7) is presented for the three main programs listed. The numbers in the following description refer to the flow chart box numbers and formula numbers of the FORTRAN listings.

1. Input, such as first guess of initial conditions, frequency of output, increment of independent variable, various end points of the independent variable, and convergence tests, is read into storage.

2. The title of the problem and the input may be printed at this step.

3. Initial values of equations are set in this box. This includes first guesses also.

4. Solution is advanced one increment in the independent variable direction. This is done by a subroutine that uses either Runge-Kutta or Adams-Moulton integration schemes. This subroutine is described in appendix C.

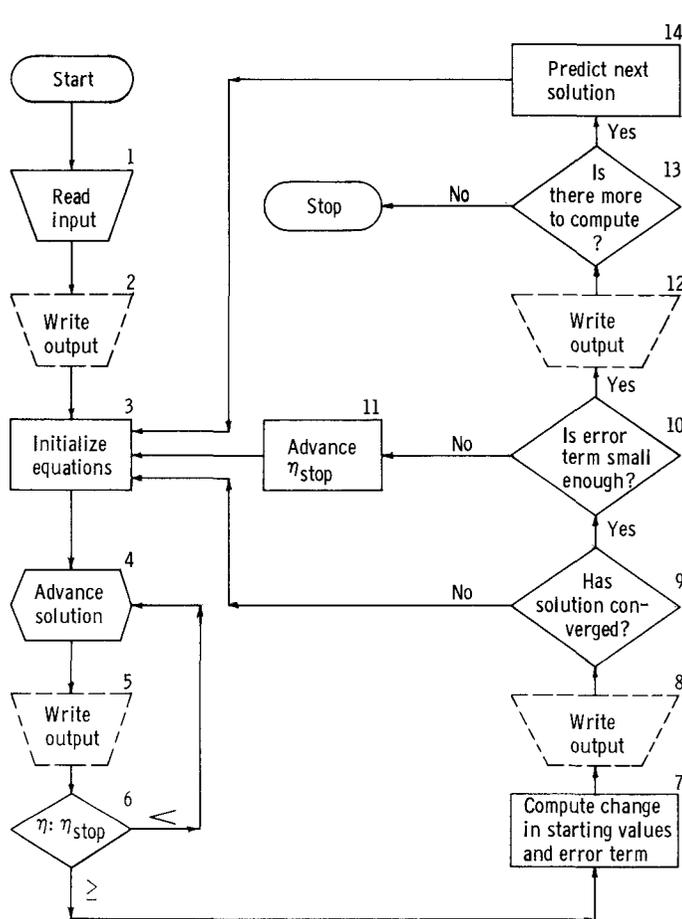


Figure 7. - General flow chart for MAIN program.

5. Output of the dependent variables may be written at this point. A test of the independent variable may be used so that output is not written at every increment.

6. If the independent variable has not reached the end point, the solution is advanced another increment.

7. Changes in starting values are computed by using equations presented in the text. Starting values are adjusted. The error term is computed.

8. Output of starting values is performed here, if desired.

9. Changes in starting values are tested to determine if convergence is realized. If not, iteration is repeated.

10. Test of the error term is made and, η_{stop} is increased if the error does not pass the test.

11. The η_{stop} is increased and the iterations are repeated.

12. Obtain error term.

13. Are more answers, such as different β , Pr , and $f''(0)$, desired? If not, stop.

14. The next solution is predicted by using a previously computed solution, extrapolation, or more input. If prediction of the next solution is good, the equations may be integrated to the largest η_{stop} directly without going through the smaller values of η_{stop} .

MAIN PROGRAM FOR EXAMPLE 1

```
DIMENSION Y(6),DY(6),ETAEND(4),TEST(4)
DOUBLE PRECISION Y,DY,H,ETA,X,B
EXTERNAL DIFF
COMMON B
1 READ (5,101) H,X,B,DELPR,ETEST
  READ (5,102) N,(ETAEND(I),TEST(I),I=1,N)
2 WRITE (6,201) H,B
  I = 1
3 PRINT = DELPR
  ETA = 0.0D0
  Y(1) = 0.0D0
  Y(2) = 0.0D0
  Y(3) = X
  Y(4) = 0.0D0
  Y(5) = 0.0D0
  Y(6) = 1.0D0
  CALL ADAMS(6,H,ETA,0,Y,DY,1,DIFF)
  WRITE (6,202) ETA,Y(1),Y(2),Y(3)
4 CALL ADAMS(6,H,ETA,1,Y,DY,1,DIFF)
  IF(ETA.LT.PRINT) GO TO 6
  PRINT = PRINT + DELPR
5 WRITE (6,202) ETA,Y(1),Y(2),Y(3)
6 IF(ETA.LT.ETAEND(I)) GO TO 4
7 DELX = (Y(5)*(1.0D0-Y(2))-Y(6)*Y(3))/(Y(5)**2+Y(6)**2)
  E = (1.0D0-Y(2))**2 + Y(3)**2
  X = X + DELX
9 IF(ABS(DELX/X).GT.TEST(I)) GO TO 3
10 IF(E.LT.ETEST) GO TO 12
11 IF(I.EQ.N) STOP
  I = I+1
  GO TO 3
12 WRITE (6,203) E
13 READ (5,103) B
  WRITE (6,201) H,B
  GO TO 3
101 FORMAT (2D10.0,D20.0,2E10.0)
102 FORMAT (I2,/, (2E10.0))
103 FORMAT (D20.0)
201 FORMAT (3H1H=,D16.8,5X,2HB=,D20.10)
202 FORMAT (4D25.8)
203 FORMAT (3H E=,E16.8)
END
```

```
C   SUBROUTINE TO COMPUTE THE DIFFERENTIAL EQUATIONS OF EXAMPLE 1
SUBROUTINE DIFF(ETA,Y,DY)
DIMENSION Y(1),DY(1)
DOUBLE PRECISION ETA,Y,DY,B
COMMON B
DY(1) = Y(2)
DY(2) = Y(3)
DY(3) = -Y(1)*Y(3) + B*(Y(2)**2-1.0D0)
DY(4) = Y(5)
DY(5) = Y(6)
DY(6) = -(Y(4)*Y(3)+Y(1)*Y(6)) + 2.0D0*B*Y(2)*Y(5)
RETURN
END
```

MAIN PROGRAM FOR EXAMPLE 2

```

DIMENSION Y(15),DY(15),ETAEND(4),TEST(4)
DOUBLE PRECISION Y,DY,H,ETA,X,Z
EXTERNAL DIFF
COMMON PR
1 READ (5,101) H,X,Z,PR,DELPR,ETEST
  READ (5,102) N,(ETAEND(I),TEST(I),I=1,N)
2 WRITE (6,201) H,PR
  I = 1
3 PRINT = DELPR
  ETA = 0.0D0
  Y(1) = 0.0D0
  Y(2) = 0.0D0
  Y(3) = X
  Y(4) = 1.0D0
  Y(5) = Z
  Y(6) = 0.0D0
  Y(7) = 0.0D0
  Y(8) = 1.0D0
  Y(9) = 0.0D0
  Y(10) = 0.0D0
  Y(11) = 0.0D0
  Y(12) = 0.0D0
  Y(13) = 0.0D0
  Y(14) = 0.0D0
  Y(15) = 1.0D0
  CALL ADAMS(15,H,ETA,0,Y,DY,1,DIFF)
  WRITE (6,202) ETA,Y(1),Y(2),Y(3),Y(4),Y(5)
4 CALL ADAMS(15,H,ETA,1,Y,DY,1,DIFF)
  IF(ETA.LT.PRINT) GO TO 6
  PRINT = PRINT + DELPR
5 WRITE (6,202) ETA,Y(1),Y(2),Y(3),Y(4),Y(5)
6 IF(ETA.LT.ETAEND(I)) GO TO 4
7 A11 = Y(7)**2 + Y(9)**2 + Y(8)**2 + Y(10)**2
  A12 = Y(7)*Y(12) + Y(9)*Y(14) + Y(8)*Y(13) + Y(10)*Y(15)
  A21 = A12
  A22 = Y(12)**2 + Y(14)**2 + Y(13)**2 + Y(15)**2
  B1 = -(Y(2)*Y(7) + Y(4)*Y(9) + Y(3)*Y(8) + Y(5)*Y(10))
  B2 = -(Y(2)*Y(12) + Y(4)*Y(14) + Y(3)*Y(13) + Y(5)*Y(15))
  DEM = A11*A22 - A21*A12
  DELX = (B1*A22-B2*A12)/DEM
  DELZ = (B2*A11-B1*A21)/DEM
  E = Y(2)**2 + Y(3)**2 + Y(4)**2 + Y(5)**2
  X = X + DELX
  Z = Z + DELZ
9 IF(ABS(DELX/X).GT.TEST(I).OR.ABS(DELZ/Z).GT.TEST(I)) GO TO 3
10 IF(E.LT.ETEST) GO TO 12
11 IF(I.EQ.N) STOP
  I = I + 1
  GO TO 3
12 WRITE (6,203) E
13 READ (5,103) PR
  WRITE (6,201) H,PR
  GO TO 3
101 FORMAT (3D10.0,3E10.0)
102 FORMAT (I2,/, (2E10.0))
103 FORMAT (E10.0)
201 FORMAT (3H1H=,D16.8,5X,3HPR=,E16.7)
202 FORMAT (6D18.8)
203 FORMAT (3H E=,E16.8)
END

```

```

C      SUBROUTINE TO COMPUTE THE DIFFERENTIAL EQUATIONS OF EXAMPLE 2
      SUBROUTINE DIFF(ETA,Y,DY)
      DOUBLE PRECISION ETA,Y,DY
      DIMENSION Y(1),DY(1)
      COMMON PR
      DY(1) = Y(2)
      DY(2) = Y(3)
      DY(3) = 2.0D0*Y(2)**2-3.0D0*Y(1)*Y(3)-Y(4)
      DY(4) = Y(5)
      DY(5) = -3.0D0*PR*Y(1)*Y(5)
      DY(6) = Y(7)
      DY(7) = Y(8)
      DY(8) = 4.0D0*Y(2)*Y(7)-3.0D0*(Y(3)*Y(6)+Y(1)*Y(8))-Y(9)
      DY(9) = Y(10)
      DY(10) = -3.0D0*PR*(Y(5)*Y(6)+Y(1)*Y(10))
      DY(11) = Y(12)
      DY(12) = Y(13)
      DY(13) = 4.0D0*Y(2)*Y(12)-3.0D0*(Y(3)*Y(11)+Y(1)*Y(13))-Y(14)
      DY(14) = Y(15)
      DY(15) = -3.0D0*PR*(Y(5)*Y(11)+Y(1)*Y(15))
      RETURN
      END

```

MAIN PROGRAM FOR EQUATIONS CONTAINING A PARAMETER

```

DIMENSION Y(9),DY(9),ETAEND(4),TEST(4)
DOUBLE PRECISION Y,DY,H,ETA,X,B
EXTERNAL DIFF
COMMON B
1 READ (5,101) H,X,B,BH,BEND,DELPR,ETEST
  READ (5,102) N,(ETAEND(I),TEST(I),I=1,N)
2 WRITE (6,201) H
  I = 1
3 PRINT = DELPR
  ETA = 0.0D0
  Y(1) = 0.0D0
  Y(2) = 0.0D0
  Y(3) = X
  Y(4) = 0.0D0
  Y(5) = 0.0D0
  Y(6) = 1.0D0
  Y(7) = 0.0D0
  Y(8) = 0.0D0
  Y(9) = 0.0D0
  CALL ADAMS(9,H,ETA,0,Y,DY,1,DIFF)
  WRITE (6,202) B,ETA,Y(1),Y(2),Y(3)
4 CALL ADAMS(9,H,ETA,1,Y,DY,1,DIFF)
  IF(ETA.LT.PRINT) GO TO 6
  PRINT = PRINT + DELPR
5 WRITE (6,203) ETA,Y(1),Y(2),Y(3)
6 IF(ETA.LT.ETAEND(I)) GO TO 4
  DEM = Y(5)**2 + Y(6)**2 + Y(8)**2 + Y(9)**2
  DELB = -((Y(2)-1.0D0)*Y(8)+Y(3)*Y(9))/DEM
  DELX = -((Y(2)-1.0D0)*Y(5)+Y(3)*Y(6))/DEM
  E = (1.0D0-Y(2))**2 + Y(3)**2
  X = X + DELX
  B = B + DELB
9 IF(ABS(DELX/X).GT.TEST(I).OR.ABS(DELB/B).GT.TEST(I)) GO TO 3
10 IF(E.LT.ETEST) GO TO 12
11 IF(I.EQ.N) STOP
  I = I + 1
  GO TO 3
12 WRITE (6,204) E
13 IF(B.GT.BEND) STOP
14 B = B + BH
  X = X - BH*(Y(5)*Y(8)+Y(6)*Y(9))/(Y(5)**2+Y(6)**2)
  GO TO 3
101 FORMAT (3D10.0,4E10.0)
102 FORMAT (I2,/,2E10.0)
201 FORMAT (3H1H=,D16.8)
202 FORMAT (3H B=,D30.16,/,4D25.8)
203 FORMAT (4D25.8)
204 FORMAT (3H E=,E16.8)
END

```

```

C      SUBROUTINE TO COMPUTE THE DIFFERENTIAL EQUATIONS OF, EQUATIONS
C      CONTAINING A PARAMETER, EXAMPLE
      SUBROUTINE DIFF(ETA,Y,DY)
      DOUBLE PRECISION ETA,Y,DY,B
      DIMENSION Y(1),DY(1)
      COMMON B
      DY(1) = Y(2)
      DY(2) = Y(3)
      DY(3) = B*(Y(2)**2-1.0) - Y(1)*Y(3)
      DY(4) = Y(5)
      DY(5) = Y(6)
      DY(6) = 2.0*B*Y(2)*Y(5)-Y(4)*Y(3)-Y(1)*Y(6)
      DY(7) = Y(8)
      DY(8) = Y(9)
      DY(9) = -(Y(1)*Y(9)+Y(7)*Y(3)) + 2.0*B*Y(2)*Y(8) + Y(2)**2-1.0
      RETURN
      END

```

APPENDIX C

INTEGRATION SUBROUTINE

Description of Flow Chart

The numbers in the following description refer to flow chart box numbers (fig. 8) and formula numbers of FORTRAN listing.

1. Test to determine if subroutine is to be initialized or if it is to advance the solution.
2. Test if subroutine is to use Runge-Kutta or Adams-Moulton integration scheme. Subroutine always uses Runge-Kutta for the first three increments.
3. Counter is initialized for Adams-Moulton scheme.
4. Counter is initialized for Runge-Kutta scheme.
5. Derivatives are evaluated at the initial value of the independent variable.
6. Counter is tested.
7. Counter is incremented by one.
8. Counter is incremented by one.
9. Counter is incremented by one.

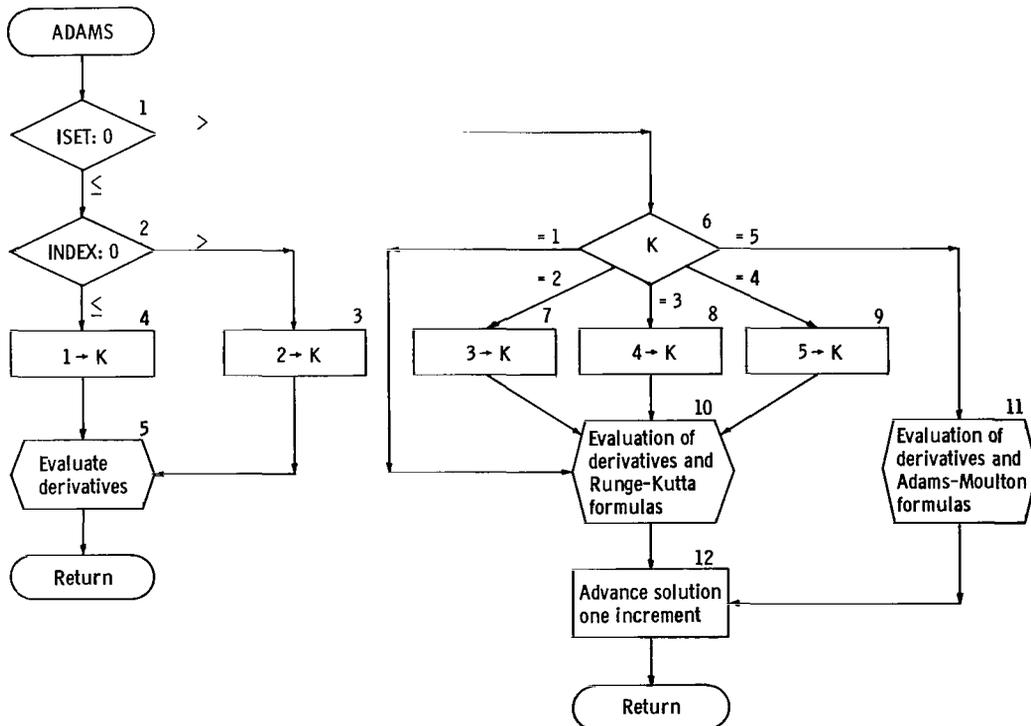


Figure 8. - Flow chart of integration subroutine.

10. Derivatives are evaluated at the proper values of the independent variable, and Runge-Kutta formulas are applied.

11. Derivatives are evaluated, and Adams-Moulton formulas are applied. Correction equation is used once for each increment.

12. Solution is advanced one increment.

This subroutine requires that a subroutine to compute the differential equations be supplied. A discussion of integration equations used in this subroutine is given subsequently.

Integration Subroutine

```

C   INTEGRATION SUBROUTINE FOR INTEGRATING SYSTEMS OF DIFFERENTIAL
C   EQUATIONS OF THE TYPE  $DY = F(X,Y)$ , BY RUNGE-KUTTA OR ADAMS-MOULTON
C   FORMULAS
C   SUBROUTINE ADAMS(N,H,X,ISET,Y,DY,INDEX,F)
C   DOUBLE PRECISION P,Y,YR,DYLL,DYLLL,DYL,DY,DYR,C2,C3,C4,X,H
C   DIMENSION Y(1),DY(1),P(24),YR(24),DYLLL(24),DYLL(24),DYL(24),DYR(
*24),C2(24),C3(24),C4(24)
1   IF(ISET.GT.0) GO TO 6
2   IF(INDEX.LE.0) GO TO 4
3   K = 2
   GO TO 5
4   K = 1
5   CALL F (X,Y,DY)
   RETURN
6   GO TO (10,7,8,9,11),K
7   K = 3
   GO TO 10
8   K = 4
   GO TO 10
9   K = 5
10  DO 1001 I=1,N
1001 P(I) = Y(I) + (H/2.0D0)*DY(I)
   CALL F(X+H/2.0D0,P,C2)
   DO 1002 I=1,N
1002 P(I) = Y(I) + (H/2.0D0)*C2(I)
   CALL F(X+H/2.0D0,P,C3)
   DO 1003 I=1,N
1003 P(I) = Y(I)+H*C3(I)
   CALL F(X+H,P,C4)
   DO 1004 I=1,N
1004 YR(I) = Y(I) + (H/6.0D0)*(DY(I)+2.0D0*C2(I)+2.0D0*C3(I)+C4(I))
   CALL F(X+H,YR,DYR)
   GO TO 12
11  DO 1101 I=1,N
1101 P(I) = Y(I) + (H/24.0D0)*(55.0D0*DY(I)-59.0D0*DYL(I)+37.0D0*DYLL
* (I)-9.0D0*DYLLL(I))
   CALL F(X+H,P,DYR)
   DO 1102 I=1,N
1102 YR(I) = Y(I) + (H/24.0D0)*(9.0D0*DYR(I)+19.0D0*DY(I)-5.0D0*DYL(I)
* +DYLL(I))
   CALL F(X+H,YR,DYR)
12  X = X+H
   DO 1201 I=1,N
   Y(I) = YR(I)
   DYLLL(I) = DYLL(I)
   DYLL(I) = DYL(I)
   DYL(I) = DY(I)
1201 DY(I) = DYR(I)
   RETURN
   END

```

Integration Formulas

The formulas described here are used in the integration subroutine given in appendix B. Let the system of n first-order differential equations to be solved be given in the form

$$\bar{y}' = \bar{f}(x, \bar{y})$$

where \bar{f} , \bar{y} , and \bar{y}' are n dimensional vectors. With initial conditions

$$\bar{y}(x_0) = \bar{y}_0$$

let h be the increment of the independent variable x , with the notation $x_j = x_0 + jh$. Then the Runge-Kutta formulas are (ref. 10):

$$\bar{y}_{j+1} = \bar{y}_j + \frac{1}{6} (\bar{k}_0 + 2\bar{k}_1 + 2\bar{k}_2 + \bar{k}_3)$$

where \bar{k}_0 , \bar{k}_1 , \bar{k}_2 , and \bar{k}_3 are n dimensional vectors and

$$\bar{k}_0 = h\bar{f}(x_j, \bar{y}_j)$$

$$\bar{k}_1 = h\bar{f}\left(x_{j+1/2}, \bar{y}_j + \frac{1}{2}\bar{k}_0\right)$$

$$\bar{k}_2 = h\bar{f}\left(x_{j+1/2}, \bar{y}_j + \frac{1}{2}\bar{k}_1\right)$$

and

$$\bar{k}_3 = h\bar{f}(x_{j+1}, \bar{y}_j + \bar{k}_2)$$

The Adams-Moulton predictor-corrector formulas of reference 10 are given by

$$\bar{y}_{j+1}^P = \bar{y}_j + \frac{h}{24} (55\bar{y}'_j - 59\bar{y}'_{j-1} + 37\bar{y}'_{j-2} - 9\bar{y}'_{j-3})$$

$$\bar{y}_{j+1}^C = \bar{y}_j + \frac{h}{24} (9\bar{y}_{j+1}^P + 19\bar{y}'_j - 5\bar{y}'_{j-1} + \bar{y}'_{j-2})$$

where

$$\bar{y}_{j+1}^{\text{P}} = \bar{f}(x_{j+1}, \bar{y}_{j+1}^{\text{P}})$$

and the superscripts **P** and **C** stand for predicted and corrected values, respectively.

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